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The Mustard Gas-Paint System Revisited

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<p>An earlier NRL report by A. Stamulis has been re-examined with more modern analytic and graphic presentation methods. The interaction of mustard gas with Navy alkylid paints as a function of temperature and wind speed was modeled as a second order polynomial with interaction terms through the use of response surface methodology techniques. The equations allowed prediction of mustard evaporation and paint absorption characteristics over the experimental range studied [30C to 50C, MPH (0.17 KPH) to 16.1 MPH (26.8 KPH)]. A recommendation is made in this report to re-examine current and planned tasks against the database of reformed WWII and post WWII reports (using modern analytic techniques such as in this report) in order that research and live testing costs may be reduced. (RL)</p>					
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EXECUTIVE SUMMARY

This report suggests that some current Navy tasks may benefit somewhat if some of the older literature is re-examined with respect to the current objectives and goals of these ongoing tasks. This report uses early 60's mustard gas Navy paint data as an example to demonstrate how older data may still remain useful to current ongoing projects when it is treated with more modern methods of data analysis. In specific the report does the following things:

1. It transforms old data suspected or shown to have relevance to current projects into graphical functions which represent the trend of this data.
2. It shows that these graphical functions can be used to provide new information capable of being used in further analyses.
3. This new information is shown to form new tables which can be analyzed with methods derived from response surface methodology to produce a more generalized model capable of more broadly representing all of the data trends.
4. This model may be used to make predictions which would be difficult to do with the original data.
5. The model - though empirical in nature - may be extremely helpful in reducing the level of experimentation required to develop the necessary data bases needed in ongoing tasks or projects.
6. The model may also suggest more meaningful experiments and or reduced experimentation to cover the goals and objectives of current ongoing tasks. Such reductions in experimentation translate into reduced costs and earlier accomplishment of the task.

The report is an outline of what can be done with old data buried in the literature, or even in old notebooks where there is a degree of reasonable completeness. Under the Data Analysis and Methodology Section it shows that the old data can be transformed into smooth functions. In the Results and Conclusions Section it shows that these smooth functions can be incorporated into a generalized model which can model all the seemingly diverse original data. It is also shown in this section that three dimensional graphs generated from the function representing the model reveal what the model looks like and give a strong feeling for the influence of the important parameters on the principal property represented by the model.

With respect to the specific illustrative example of this report for the interaction of mustard gas with paint the following results and conclusions were obtained:

- a) Models were developed which represented mustard paint interactions over a range of temperatures and wind speeds.

b) These models represented the effect of temperature and wind speed on the mustard evaporation time and the sorption power of the paint for mustard liquid.

c) The sorption power model shows that fresh paint absorbs mustard more readily than aged paint.

d) The sorption power model also shows that temperature promotes absorption of mustard into paint while wind speed lessens absorption into the paint.

e) The evaporation models show that both temperature and wind speed promote effective evaporation of mustard and that these evaporation times are reasonably tracked by the model over the experimental range of temperature and wind speed.

THE MUSTARD GAS-PAINT SYSTEM REVISITED

INTRODUCTION

CW decontamination is a costly and time-consuming operation which is both manpower-intensive and manpower-constrictive. The need for decontamination may be properly addressed when the type and concentration of the deposited chemical agent are known. Weathering becomes a suitable alternative to decontamination when the environmental parameters of temperature, incident radiant energy and wind speed are shown to promote favorable evaporation of the deposited chemical agent with respect to operational considerations.

Mustard gas (HD) is a favorite chemical agent for use as a laboratory model of a chemical agent. While it lacks the killing power of the exotic nerve agents by at least an order of magnitude, its persistence and ability to cause disfiguring life-long injuries and incapacitation to survivors is well-known. It also has the advantage of tying up significant numbers of personnel to administer to the injured individuals as opposed to merely setting aside the dead for burial. It (HD) also is one of the more intractable agents to decontaminate in addition to being relatively persistent. Mustard, in spite of its long history, remains the agent of choice in practical studies of decontamination and weathering effects.

One of the early laboratory weathering studies on mustard gas was done at this Laboratory in 1961 (1) by A. Stamulis. This report looked at the evaporation of HD from both fresh and aged painted Navy marine surfaces as a function of temperature and wind speed under controlled laboratory conditions. In this report, Stamulis treated the evaporation process as being divided into two characteristic regions: (a) the exposed liquid surface region and (b) the sorbed liquid (into the paint) region. Most importantly, Stamulis provided data tables for his controlled experiments which are most worthy of being re-examined in the light of new methodologies.

This report will revisit this data and attempt to develop relations which may be useful for those concerned with the weathering properties of the mustard-paint system. If the results presented in this report have some merit or application or if the methods used will be useful in making practical guesses or judgments with respect to weathering decisions, then this report can be justified. An important objective of this report is to be able to predict the percent of mustard evaporated from paint surfaces as a function of temperature, wind speed and time from a minimum of experimental data. In order

to achieve this objective a combination of analytic methods will be used which will (1) reduce Stamulis's evaporation curve results to a series of two parameter equations and (2) develop an empirical equation which will show the effect of temperature and wind speed using the evaporation half life parameter developed from the two parameter evaporation curve plots (Michaelison-Menten plots).

This report also features the use of response surface methodology (RSM) methods to extract relationships from the experimental data array. In order to make progress rapidly in the use of a new method or technique it is necessary to (1) gain a knowledge of how to apply the given method or technique to the problem of interest and (2) gain an understanding of the principles and theory on which the method/technique is based. It is the writer's contention that the two are to some degree mutually exclusive in that a thorough understanding of the principles on which a particular technique is based is not absolutely necessary to its initial application. This report will not attempt to explain the statistical theory behind the use of RSM but, rather, quickly expose the reader to the tools by which he may organize/plan/interpret his experiments. The reference section contains information on the statistical theory behind the development of RSM (2,3). Upon completion of these operations, the reader will be left with a reasonable view of mustard evaporation as a function of environmental parameters and paint type.

DATA ANALYSIS AND METHODOLOGY

Michaelison-Menten Analysis

Preliminary analysis of Stamulis's data showed that the sorbed agent data could be reasonably well represented by a hyperbolic equation of the type

$$ZEV = (t/(t + K)) * ZEV(MAX)$$

where K and ZEV(MAX) are constants to be determined by the data fit, t = time in hours and ZEV = percent mustard evaporated at time t. The constant K represents the half life of the evaporation process, that is the point in time at which one half of the deposited chemical agent has disappeared. The constant ZEV(MAX) is the percent of agent evaporated at infinite time which ideally should be 100% in value.

There are three ways to plot the experimental data to such an equation in order to obtain these parameters (4). A simple least squares fit computer program adapted from a literature Fortran program has been used to show the difference between these plot results. The three methods are (1) the Lineweaver-Burk method, (2) the Michaelison-Menten method and (3) the Eadie-Hofstee method. The Lineweaver-Burk method plots $1/ZEV$ vs $1/t$. The slope is $K/ZEV(MAX)$ while the intercept with the y axis is $1/ZEV(MAX)$ and with the x axis is $-1/K$. A problem with this method is that data points with small values which are inaccurate are too strongly weighted when reciprocals are plotted. The Michaelison-Menten method plots t/ZEV vs t . The slope of this plot is $1/ZEV(MAX)$ and the intercept with the y axis is $K/ZEV(MAX)$. In the Eadie-Hofstee method ZEV is plotted against ZEV/t . The slope is $-K$ and the intercept with the y axis is $ZEV(MAX)$ and with the x axis is $ZEV(MAX)/K$. The method selected in this report was the Michaelis-Menten method since present

experience shows it to give the most consistent and reliable results over the observed range of data points. For example, Table 1 shows the results obtained by least squares using the three methods for two quite different data files. The Lineweaver-Burke Method invariably gives the lowest values of variance and standard deviation but the values of the parameters are sometimes far afield of the expected values. The Eadie-Hofstee Method gives values which are more in line with expectations but the variance and standard deviation are almost always significantly greater than for the Michaelson-Menten Method. Figure 1 is an example of the data fit to the Michaelis-Menten relation where K was found to be 0.3616 and the value of $\Sigma EV(\text{MAX})$ was found to be 100%. Plots of Stamulis's data at various temperatures and windspeeds were done by computer and reasonable conformity to the relation was found. The values of K were set aside for each condition of temperature and wind speed.

Response Surface Methodology

A useful RSM design adaptable to Stamulis's data is the face or side-centered design (we will not attempt the pros and cons of one design vs another in this report). This design produces a polynomial which contains a constant term, linear terms, quadratic terms and cross-product terms and is of the form:

$$Y = B_0 + \sum_{i=1}^n B_i X_i + \sum_{i=1}^n B_{ii} X_{ii}^2 + \sum_{i=1}^n \sum_{j>i} B_{ij} X_i X_j$$

In order to develop the coefficients of the above polynomial it is necessary to run experiments in the independent variables (x's) and observe the dependent variables (y's). To successfully accomplish this goal requires an experimental 'recipe' which, when used with an appropriate array, will allow computer solution of the desired coefficients. The coefficients obtained are a least squares-like fit of the data to the polynomial. It should again be emphasized that the polynomial obtained is not a representation of the 'natural law' which is at work. It will, however, represent the variation of the response variables (y's) to the independent variables (x's) perhaps as well as the natural law itself over the same range of independent variables from which the polynomial was obtained were the natural law adequately known.

In the case of 2 variables, the number of experiments for single runs without duplication should be 9 (4 for each corner of the square plus 4 center points in each side plus the center of the square). The data array required for a polynomial containing 2 independent variables with interactions is shown in Table 2. Note that the x's are given in coded form. This is an aid in both conforming to the experimental design and in the rational solution of the equations set up for determining the coefficients. The 2 variable situation is probably one of the most common encountered in the laboratory and its inclusion here will make a reasonable example. The half matrix representing the normal equations is shown in Table 3. The specific relations for B1, B2 and B12 are shown together with the full reduced matrix which must be inverted to solve for B0, B11 and B22.

One of the principal thrusts behind the intent to produce a statistical equation is the development of a function by means of which surface plots and/or contour maps may be generated. Such maps will greatly aid the experimenter in obtaining a grand view of his experimental results over the range of interest and also, perhaps, to make some limited predictions. Figure 2, then, summarizes the operations and goals described in this section. Examples of RSM methods and software used by the author relevant to this paper may be found in earlier reports (5,6,7,8).

III. RESULTS

Tabulation of Data Matrix (RSM Analysis):

Table 4 is a summary of Stamulis's evaporation data taken at a variety of conditions and on several types of Navy paints both fresh and aged. The conditions ranged from 30°C to 50°C in temperature and from 0.1 to 16.1 miles per hour in wind speed. The paints used were of the alkyd resin type, both fresh and aged (eight years old). Also included in the Table are data computed from the Michaelson-Menten plots which were recorded as corresponding values of K and ZEV(MAX) for each condition of temperature and wind velocity. Table 4 provides the basis for the development of Tables 5 and 6 which contain selected and interpolated values of the independent and dependent (response) variables to conform to the orthogonal side centered statistical design mentioned earlier. Table 5 summarizes the extracted data for the aged paint experiments while Table 6 presents the mustard evaporation data from freshly painted surfaces. It should be noted that Stamulis's data mostly conformed to the side centered statistical design with only minimal interpolations being needed to arrive at the 8.1 mph condition required for the orthogonality condition instead of the 6.1 mph data documented in Stamulis's report. In the design it should be noted that the dependent variable is taken as the logarithm of the half life of the given mustard-paint system. Such a dependent variable transformation allows a much closer correlation with the independent variables of the experimental design. Also included in Tables 5 and 6 are data on Stamulis's "sorbing power coefficient", Ksp. These data were also entered for a total of 4 separate equation determinations. Stamulis defines his sorption power coefficient as "the ease with which a given paint film absorbs mustard gas under given evaporation conditions". No transformation of the response variable was required for the sorption power coefficients.

Development of Descriptive Equations:

Table 7 summarizes the coefficients obtained by solution of the four systems of normal equations represented by the matrices of Table 2 and 3 together with the response variable data of Tables 5 and 6. These coefficients are substituted as appropriate in the given descriptive equation. As mentioned in the earlier section, these equations may now be used to (1) generate three dimensional surfaces and/or contour maps and (2) make predictions of experimental behavior covered by the experimental design. It must be emphasized that experimental designs of this type cannot be used to make extrapolations beyond the region enclosed by the design.

Predictive Results vs Actual Data:

Table 8 presents the results of computing the percent mustard evaporated using K derived from the descriptive two variable equations of the previous section, one equation representing aged paint and the other the fresh paint relation. Only the K value was used in the computations of the percent evaporated as ZEV(MAX) was set to 100%. Thus, coded values of temperature and windspeed were substituted into the descriptive equation to generate the K value. The K value was substituted into the Michaelson-Menten hyperbolic relation assuming ZEV(MAX) = 100% and the data values calculated for the time intervals indicated in Table 8. In spite of the fact that some of Stamulis's data was rather scanty and frankly incomplete, the agreement between the predicted results and the original data is reasonable in most cases and gives some confidence in looking at the general appearance of the three dimensional surface function generated by the descriptive equation.

Evaporation and the Paint Sorption Power Coefficient:

Stamulis has defined a paint sorption power coefficient based on a comparison of his experimental evaporation data with his "dry line" curve. No attempt will be made here to go into the details of his "dry line" concept but rather to point out that a straight forward analysis of the evaporation from paint films as opposed to evaporation from bare metal surfaces leads more clearly to the same results for the value of paint sorption power coefficients as he obtained in his report with no graphical geometry required in the analysis.

Figure 3 is a diagram of chemical agent evaporation from a bare metal as opposed to a paint film. The time required to evaporate 100% of the agent from the bare metal, t' , is used to estimate the value of ZEV'. It is clear that

$$ZEV' = (t'/(t' + K))100 \text{ or } ZEV/100 = t'/(t' + K)$$

If the sorption coefficient is defined as $Ksp = (100 - ZEV')/100$, Ksp may be reduced to $Ksp = 1 - ZEV'/100$. Upon substitution into the above equation one obtains

$$Ksp = K/(t' + K)$$

Comparison of sorption power coefficients calculated directly from mustard-paint film half lives showed an agreement of $\pm 10\%$ with Stamulis's original Ksp values without the use of the any graphical geometry for the computation.

Three Dimensional Graphics:

Figures 4 through 8 show the power of three dimensional graphics giving a broad visual view of exactly how a function is behaving over the desired range of interest. Figures 4 and 5 compare the behavior of mustard evaporating from aged paint with evaporation from fresh paint. The x-axis represents the effect of temperature and the y-axis the effect of wind speed while the z-axis is the normalized effect of these two independent variables on logarithm of the mustard half-life. Figure 6 is a plot of the difference between the logarithms of the half-lives of the aged and fresh painted surfaces vs temperature and

wind speed. Where values on the z-axis are low it indicates that curve differences are small and vice versa. It would appear that the paints (aged vs fresh) show the greatest differences at higher wind speeds since the difference in the logarithms of the half-lives is highest at the greater wind speeds.

Figures 7 and 8 compare the paint sorption power coefficients as affected by temperature and wind speed for aged paint vs fresh paint. Inspection of Table 7 and comparison of the figures show vividly how the fresh paint more effectively absorbs the mustard as against the aged paint and how an increase in temperature promotes increased sorption of the mustard gas by the paint in both cases. As expected, increased wind speed decreases the sorption power coefficient for both aged and fresh paints. In the case of these alkyd type paints while temperature increases the rate of evaporation, it also promotes the penetration of the chemical agent into the paint. Moreover, the aging of alkyd type paints appears to inhibit the penetration of the chemical agent into the paint film.

IV. CONCLUSIONS

a) Models can be developed which represent the dependence of important system properties over a range of independent variables when properly selected archival data is used as a basis for these models.

b) The exemplary models of this report represent the effect of temperature and wind speed on the mustard evaporation time and the sorption power of the paint for mustard liquid.

c) The sorption power model shows that fresh paint absorbs mustard more readily than aged paint.

d) The sorption power model also shows that temperature promotes absorption of mustard into paint while wind speed lessens absorption into the paint.

e) The evaporation models show that both temperature and wind speed promote effective evaporation of mustard and that these evaporation times are reasonably well tracked by the model over the experimental range of temperature and wind speed.

V. RECOMMENDATIONS

A large database of investigated chemical agent systems lies in the variety of government reports published over the years. While these reports are accessible through DOD and NTIS services etc. many reports such as the one examined here may have new value if re-examined within the context of new analytic methods or methodologies. Since the costs of live agent tests and research in general have soared in recent years, it might be useful to critically examine the older reports in a systematic manner using the newer analytic methods presented here to reduce some of the expensive and time consuming live agent testing to which the armed services are committed. In specific and to the point:

1. That a task be set up to critically review the content of WWII and post WWII chemical agent work to determine the merit of this work against the requirements and planned research addressed by current ongoing or planned CBR tasks.

2. That the more useful and relevant of these reports be reformatted using methods similar to the ones used in this report in order to both extract the maximum amount of information and reduce the cost of additional live agent testing- especially if it is established that similar work has already been accomplished in this earlier literature relevant to these CBR tasks.

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REFERENCES

1. Stamulis, A., "Studies of the Mustard Gas-Paint System, Part I- The Evaporation of Mustard Gas From Paint Films," NRL Report 5712, 1962.
2. Davies, O.L., Editor, "The Design and Analysis of Industrial Experiments," Hafner Publishing Company, New York, 2nd Edition, 1967.
3. Cochran, W.G. and Cox, G.M., "Experimental Designs," Wiley and Sons, New York 2nd Edition, 1957.
4. Jur S, P., "Computer Software Application in Chemistry," John Wiley & Sons, New York, 1986.
5. Little, R. and Shirley, J., "The Application of Statistics to Laboratory Decontamination Experiments," NRL Memorandum Report 5780, 1986.
6. Little, R. and Shirley, J., "Decontamination Part I: Simulant Removal as Indexed by Contact Angle Measurements," NRL Memorandum Report 5786, 1986.
7. Little, R. and Shirley, J., "Decontamination Part II: Simulant Removal as Influenced by Substrate and Surfactant," NRL Memorandum Report 5803, 1986.
8. Little, R. and Shirley, J., "Decontamination Part III: Simulant Emulsification as a Function of Surfactant and Ultrasonic Energy Input," NRL Memorandum Report 5800, 1986.

Table 1: Least Squares Data Plots for the Three Methods

HD.10.STAM.ETK		HD.33.STAM.ETK	
S	V	S	V
1.5	30.1	1	11
2	35.6	2	22.5
3	48	3	35.5
4	59.5	5	62.4
5	68.6	6	74.9
6	73.1	7	80
24	90.5	24	87
48	94.2	48	88.2

LINEWEAVER-BURK METHOD		LINEWEAVER-BURK METHOD	
ZEV(MAX) = 116.364527		ZEV(MAX) = 333.171971	
K = 4.27860016		K = 28.2869931	
VARIANCE = 2.2535524E-09		VARIANCE = 1.22701418E-03	
STN DEV = 4.74715957E-05		STN DEV = 1.22701418E-03	

MICHEALIS-MENTEN METHOD		MICHEALIS-MENTEN METHOD	
ZEV(MAX) = 100.493319		ZEV(MAX) = 98.6486888	
K = 2.95253882		K = 4.42648385	
VARIANCE = 5.09142197E-06		VARIANCE = 2.14812686E-04	
STN DEV = 2.25641795E-03		STN DEV = .0146564895	

EADIE-HOFSTEE METHOD		EADIE-HOFSTEE METHOD	
ZEV(MAX) = 106.271227		ZEV(MAX) = 94.0696557	
K = 3.49248494		K = 3.8328406	
VARIANCE = 6.17870316		VARIANCE = 278.916323	
STN DEV = 2.48569973		STN DEV = 16.7007881	

Table 2. Side-Centered Two Variable Design

	Design Matrix				Graphic Representation		
	N	X ₁	X ₂	Y			
Corners	1	1	1	Y ₁		X	X
	2	1	-1	Y ₂			X
	3	-1	1	Y ₃		X	
	4	-1	-1	Y ₄	X ₂	X	X
Side of Face Centered Pts	5	1	0	Y ₅			
	6	-1	0	Y ₆			
	7	0	1	Y ₇		X	X
Center Point	8	0	-1	Y ₈			
	9	0	0	Y ₉		X ₁	

Table 3. Solution of Normal Equations

N	ΣX_1	ΣX_2	ΣX_1^2	ΣX_2^2	$\Sigma X_1 X_2$	ΣY
	ΣX_1^2	$\Sigma X_1 X_2$	ΣX_1^3	$\Sigma X_1 X_2^2$	$\Sigma X_1^2 X_2$	$\Sigma X_1 Y$
		ΣX_2^2	$\Sigma X_1^2 X_2$	ΣX_2^3	$\Sigma X_1 X_2^2$	$\Sigma X_2 Y$
			ΣX_1^4	$\Sigma X_1^2 X_2^2$	$\Sigma X_1^3 X_2$	$\Sigma X_1^2 Y$
				ΣX_2^4	$\Sigma X_1 X_2^3$	$\Sigma X_2^2 Y$
					$\Sigma X_1^2 X_2^2$	$\Sigma X_1 X_2 Y$
9	0	0	6	6	0	ΣY
	6	0	0	0	0	$\Sigma X_1 Y$
		6	0	0	0	$\Sigma X_2 Y$
4p			6	4	0	$\Sigma X_1^2 Y$
				6	0	$\Sigma X_2^2 Y$
					4	$\Sigma X_1 X_2 Y$

$$B_1 = \Sigma X_1 Y / 6$$

$$B_2 = \Sigma X_2 Y / 6$$

$$B_{12} = \Sigma X_1 X_2 Y / 4$$

Note:

Relations for Linear and Intereaction Coefficients

$$9 \quad 6 \quad 6 \quad \Sigma Y$$

$$6 \quad 6 \quad 4 \quad \Sigma X_1^2 Y$$

$$6 \quad 4 \quad 6 \quad \Sigma X_2^2 Y$$

Note:

Invert Matrix to Solve for B₀ and Second Order Coefficients

Table 4
Wind Tunnel Evaporation of HD from Paint Films

Temp. and Age of Paint	Sample No.	Paint Type	Original Wt of HD on Paint Surface (g)	Wind Speed (mph)	Paint Film Thickness (mils)	t _{hrs} ^a (min)	Evaporated HD (%)															High-Hum. Parameters								
							5 min	10 min	15 min	20 min	25 min	30 min	40 min	50 min	60 min	90 min	120 min	150 min	180 min	240 min	300 min	330 min	360 min	420 min	480 min	1360 min	1380 min	1440 min	2880 min	ZEV
30°C - 8-Year-Old Paint	7	20A	0.0334	0.1	2.8	233	-	-	-	-	-	-	-	-	24.0	-	48.2	-	70.4	85.0	87.0	-	89.2	-	-	-	95.5	99.1	102.7	1.639
	8	5H	0.0463	0.9	3.0	200	-	-	-	-	-	-	-	-	50.5	-	70.0	-	80.5	87.0	93.1	-	-	-	95.9	-	97.0	99.4	100.8	.7121
	9	5H	0.0362	6.1	3.0	70	-	-	-	-	-	-	-	-	88.1	-	91.8	-	92.3	-	-	-	94.2	-	-	-	-	-	95.5	.0879
	10	20A	0.0447	16.1	2.0	55	-	-	-	-	-	84.3	-	-	97.1	-	-	-	-	96.6	97.5	-	-	-	-	-	-	-	98.3	.0521
40°C - 8-Year-Old Paint	11	5H	0.0410	0.1	3.0	165	-	-	-	-	-	-	-	-	25.0	-	49.0	-	74.9	76.8	-	-	86.1	-	-	-	96.8	99.0	103.2	1.807
	12	20A	0.0396	0.9	4.0	70	-	-	-	-	-	-	-	-	80.3	-	94.4	-	-	94.7	-	-	-	-	-	99.2	-	100.0	.1961	
	13	5H	0.0365	6.1	3.1	28	-	-	-	-	-	92.6	-	-	96.4	-	98.6	-	-	-	-	99.5	-	-	-	-	-	-	100.2	.0384
	14	5H	0.0753	16.1	3.0	25	-	-	-	-	-	91.1	-	-	96.3	-	-	-	97.7	99.5	-	-	-	-	-	-	-	-	100.3	.0506
50°C - 8-Year-Old Paint	15	5H	0.0490	0.1	5.1	82	-	-	-	-	-	-	-	-	-	-	81.6	-	-	89.9	-	-	91.8	-	-	-	-	-	97.9	.3856
	16	20A	0.0604	0.9	5.0	30	-	41.4	-	72.5	-	87.7	88.9	91.4	92.1	-	95.4	-	-	96.9	-	-	-	-	-	-	-	-	100.4	.1177
	17	20A	0.0586	6.1	3.0	25	-	51.9	-	85.3	-	90.8	92.2	-	-	95.4	-	95.4	-	97.3	-	-	-	-	-	-	-	-	99.3	.0787
	18	5H	0.0764	16.1	3.0	10	-	82.5	-	89.5	-	91.6	-	-	95.2	-	97.8	-	-	99.4	-	-	-	-	-	-	-	-	100.4	.0452
30°C - Fresh Paint	19	20A	0.0242	0.1	5.0	213	-	-	-	-	-	-	-	-	-	30.1	35.6	-	48.0	59.5	68.6	-	73.1	-	-	90.5	94.2	100.5	2.952	
	20	5H	0.0411	0.9	5.0	93	-	-	-	-	-	-	-	-	44.3	-	-	-	86.4	-	91.0	-	-	-	-	96.6	99.3	100.8	.852	
	21	5H	0.0384	6.1	3.0	55	-	-	-	-	-	-	-	-	79.0	-	87.0	-	-	94.0	-	-	-	-	-	-	-	-	100.6	.2894
	22	20A	0.0579	16.1	6.0	25	-	-	-	-	-	-	-	-	-	-	-	-	-	93.4	-	-	95.9	-	-	-	-	-	101.3	.3394
40°C - Fresh Paint	23	5H	0.0337	0.1	5.0	-	-	-	-	-	-	-	-	-	-	-	58.0	-	-	82.0	-	87.0	-	-	-	92.2	-	-	95.8	.8658
	24	20A	0.0473	0.9	5.0	45	-	-	-	-	-	-	-	-	82.0	-	90.0	-	-	94.7	-	-	-	-	-	97.3	-	-	98.0	.1844
	25	5H	0.0411	6.1	6.0	-	-	-	-	-	-	83.0	-	-	89.1	-	-	91.5	-	94.4	96.0	-	-	-	-	-	-	-	97.4	.1072
	26	5H	0.0749	16.1	6.0	25	-	-	-	-	-	-	-	-	85.0	-	-	-	-	-	-	-	98.7	-	-	-	-	-	102.0	.2000
50°C - Fresh Paint	27	5H	0.0525	0.1	5.0	39	-	12.0	-	22.5	-	31.5	38.0	43.5	48.2	-	69.5	-	77.0	-	-	-	-	-	-	87.2	-	-	90.5	.8650
	28	5H	0.0503	0.9	5.0	25	11.0	21.0	31.0	42.0	47.0	-	-	-	78.9	-	87.1	-	-	-	-	-	-	-	-	-	-	-	100.	.3616
	29	5H	0.0706	6.1	14.0	20	17.0	34.0	46.0	56.0	-	-	-	-	73.5	-	80.7	-	-	-	-	-	-	-	-	-	-	-	92.2	.2769
	30	5H	0.0649	16.1	14.0	10	-	57.3	-	67.0	-	71.0	73.2	74.9	77.8	-	81.4	-	83.5	-	-	-	-	-	-	-	-	-	86.0	.1046
30°C - 8-Year-Old Paint	31	5H	0.0310	0.1	2.7	303	-	-	-	-	-	-	-	-	21.3	-	35.0	-	51.5	-	89.3	-	-	89.7	-	95.1	-	-	109.5	3.018
	32	5H	0.0370	0.1	5.1	330	-	-	-	-	-	-	-	-	17.3	-	28.5	-	40.5	-	76.2	-	79.7	87.0	-	96.8	-	-	119.3	4.584
	33	5H	0.0458	0.1	13.6	411	-	-	-	-	-	-	-	-	11.0	-	22.5	-	35.5	-	62.4	-	74.9	80.0	-	87.0	88.2	-	98.6	4.426
30°C - Fresh Paint	34	20A	0.0344	0.1	5.0	247	-	-	-	-	-	-	-	-	-	-	27.0	-	-	48.8	59.3	-	65.7	-	-	90.4	-	-	104.6	4.364
	35	20A	0.0371	0.1	8.0	125	-	-	-	-	-	-	-	-	-	-	25.8	-	-	41.8	49.6	-	54.7	-	-	76.8	-	-	91.0	4.459
	36	20A	0.0422	0.1	13.0	119	-	-	-	-	-	-	-	-	-	-	23.5	-	-	32.9	38.9	-	41.7	-	-	61.6	-	-	76.8	5.035

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Table 5. Eight Year Paint Data Used in Design

STAMULIS EXP. NO.	TEMP	X ₁	WIND	X ₂	Y	t1/2	Logt1/2	k _{sp}
18	50	1	16.1	1	Y(1)	.0451	-1.346	.23
15	50	1	0.1	-1	Y(2)	.385	-.4145	.23
10	50	1	16.1	1	Y(3)	.0521	-1.283	.08
07	30	-1	0.1	-1	Y(4)	1.640	.2148	.15
*	50	1	8.1	0	Y(5)	(.0720)	-1.143	(.18)est.
*	30	-1	8.1	0	Y(6)	(.0808)	-1.092	(.12)est.
14	40	0	16.1	1	Y(7)	.0506	-1.296	.13
11	40	0	0.1	-1	Y(8)	1.807	.2570	.35
*	40	0	8.1	0	Y(9)	(.0408)	-1.389	(.13)est.

* = interpolated row values from data

Table 6. Fresh Paint Data Used in Design

STAMULIS EXP. NO.	TEMP	X ₁	WIND	X ₂	Y	t1/2	Logt1/2	k _{sp}
18	50	1	16.1	1	Y(1)	.1046	-.9805	.23
27	50	1	0.1	-1	Y(2)	.8650	-.0630	.63
22	30	-1	16.1	1	Y(3)	.3394	-.4693	.39
19	30	-1	0.1	-1	Y(4)	2.952	.4701	.33
*	50	1	8.1	0	Y(5)	(.2424)	-.6155	(.48)est.
*	30	-1	8.2	0	Y(6)	.2994	-.5237	(.23)est.
26	40	0	16.1	1	Y(7)	.2000	-.6990	.32
40	0	0	0.1	-1	Y(8)	.8658	-.0626	.80
*	40	0	8.1	0	Y(9)	(.1258)	-.9003	(.40)est.

* = interpolated row values from data

Table 7. Summary of Equation Coefficients

COEFFICIENT	AGED PAINT		FRESH PAINT	
	Y=LogK	Y = K _{sp}	Y = LogK	Y = K _{sp}
B ₀	-1.2579	0.1550	-0.8492	0.4343
B ₁	-0.1239	0.04833	-0.1584	0.0650
B ₂	-0.6637	-0.04833	-0.4366	-0.1367
B ₁₁	0.00914	0.03000	0.2284	-0.1136
B ₂₂	0.6072	0.0600	0.4172	0.0914
B ₁₂	0.1416	0.0175	-0.0260	-0.1150
MODEL EQUATION: $Y = B_0 + B_1X_1 + B_2X_2 + B_{11}X_1^2 + B_{22}X_2^2 + B_{12}X_1X_2$				
X ₁ = Coded Temperature		X ₂ = Coded Wind Speed		
$X_1 = \frac{C-40}{10}$		$X_2 = \frac{WS - 8.1}{8}$		

Table 8. Actual Data vs. Predictive Results (in Parentheses)

TEMP (°C)	WIND (MPH)	PERCENT EVAPORATED AT INDICATED TIME IN HOURS									
		0.5	1	2	3	4	5	24	48		
30	0.1	(20.3)	24.0(33.8)	48.2(50.5)	70.4(60.5)	85.0(67.1)	87.0(71.9)	95.5(92.4)	99.1(96.1)		
	0.9	(28.6)	50.5(44.5)	70.0(61.6)	80.5(70.6)	87.0(76.2)	91.1(80.9)	97.0(95.1)	99.4(97.5)		
	6.1	(79.3)	88.1(88.5)	91.8(93.9)	92.3(95.8)	(96.8)	(97.4)	94.2(97.9)	(99.2)		
	16.1	84.3(91.4)	97.1(95.5)	(97.7)	(98.4)	96.6(98.8)	(99.1)	(99.8)	(99.9)		
40	0.1	(32.7)	35.0(49.2)	49.0(66.0)	74.9(74.4)	76.8(79.5)	(82.9)	96.8(95.9)	99.0(97.9)		
	0.9	(42.4)	80.3(59.6)	94.4(74.7)	(81.6)	94.7(85.5)	(88.1)	99.2(97.2)	(98.6)		
	6.1	92.6(85.0)	96.4(91.9)	98.6(95.8)	(97.1)	(97.8)	(98.3)	(99.6)	(99.8)		
	16.1	91.1(91.2)	96.3(95.4)	(97.6)	97.7(98.4)	99.5(98.9)	(99.0)	(99.8)	(99.9)		
50	0.1	(46.9)	(63.9)	81.6(78.0)	(84.1)	89.9(87.6)	(89.8)	91.8(91.4)	(97.7)		
	0.9	87.7(56.5)	92.1(72.2)	95.4(73.9)	(88.6)	96.9(91.2)	(92.8)	(94.0)	(98.4)		
	6.1	90.8(88.9)	(94.1)	95.4(97.0)	(98.0)	97.3(98.5)	(98.8)	(99.0)	(99.7)		
	16.1	91.6(90.6)	95.2(95.0)	97.8(97.5)	(98.3)	99.4(98.7)	(99.0)	(99.1)	(99.8)		
30	0.1	(17.4)	(29.6)	35.6(45.7)	48.0(55.8)	59.5(62.8)	68.0(62.8)	73.1(7.6)	90.5(91.0)	94.2(95.3)	
	0.9	(21.8)	44.3(35.7)	(52.6)	86.4(62.5)	(69.0)	91.0(73.5)	(76.9)	96.6(91.0)	99.3(96.4)	
	6.1	(51.3)	79.0(67.8)	87.0(80.8)	(86.3)	94.0(89.4)	(91.3)	(92.7)	(98.1)	(99.0)	
	16.1	(58.2)	(73.6)	(84.8)	(89.3)	93.4(91.8)	(97.3)	95.9(94.4)	(98.5)	(99.2)	
40	0.1	(33.1)	(49.7)	53.0(66.4)	(74.8)	82.0(79.8)	(83.2)	(85.6)	92.2(96.0)	(97.9)	
	0.9	(39.6)	82.0(56.9)	90.0(72.4)	(79.8)	(84.0)	94.7(86.8)	(88.7)	97.3(96.9)	(98.4)	
	6.1	83.0(72.1)	89.1(83.8)	(91.2)	(91.9)	94.4(95.4)	96.0(96.3)	(95.9)	(97.2)	(99.6)	
	16.1	(78.7)	85.0(88.1)	(91.7)	(95.7)	(96.7)	(97.4)	98.7(97.8)	(99.4)	(99.7)	
50	0.1	(28.9)	48.7(44.8)	69.5(61.9)	77.0(70.9)	(76.4)	(80.2)	(81.0)	87.2(95.1)	(97.5)	
	0.9	(35.1)	78.9(52.0)	87.1(68.4)	(76.5)	(81.2)	(84.4)	(86.7)	(98.1)	(98.1)	
	6.1	(68.9)	73.5(81.6)	80.7(89.9)	(91.0)	(95.7)	(95.7)	(96.4)	(99.5)	(99.5)	
	16.1	71.0(77.4)	77.8(87.2)	81.4(93.2)	83.5(95.3)	(96.5)	(97.2)	(97.6)	(99.2)	(99.7)	

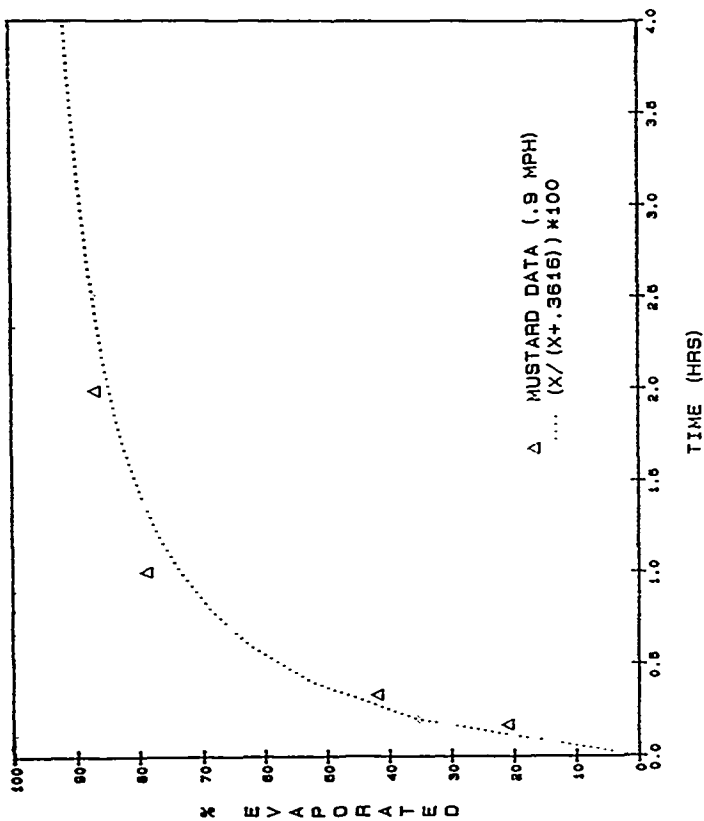


FIGURE 1. Evaporation of Mustard from Fresh Paint: Comparison of Equation and Experimental Data Points.

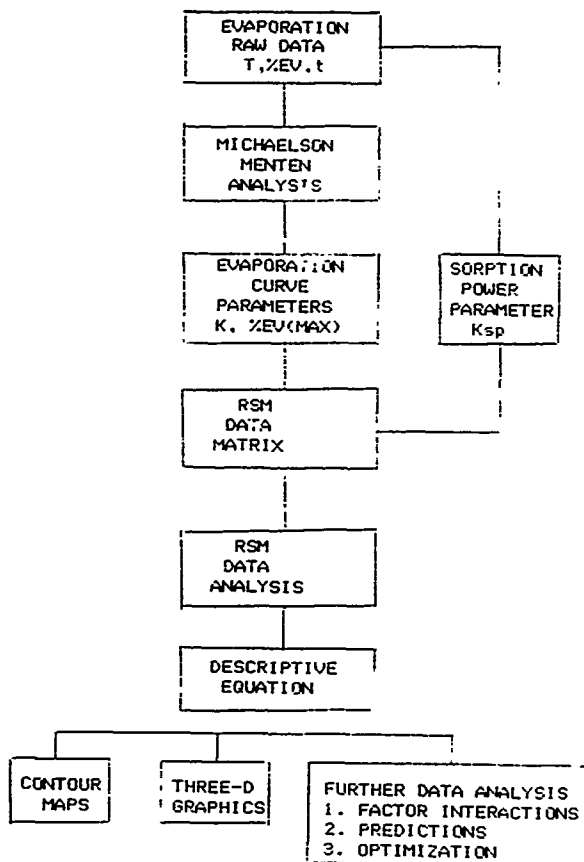


Figure 2. Treatment of Experimental Data and Analysis

EVAPORATION FROM METAL VS ALKYD PAINT

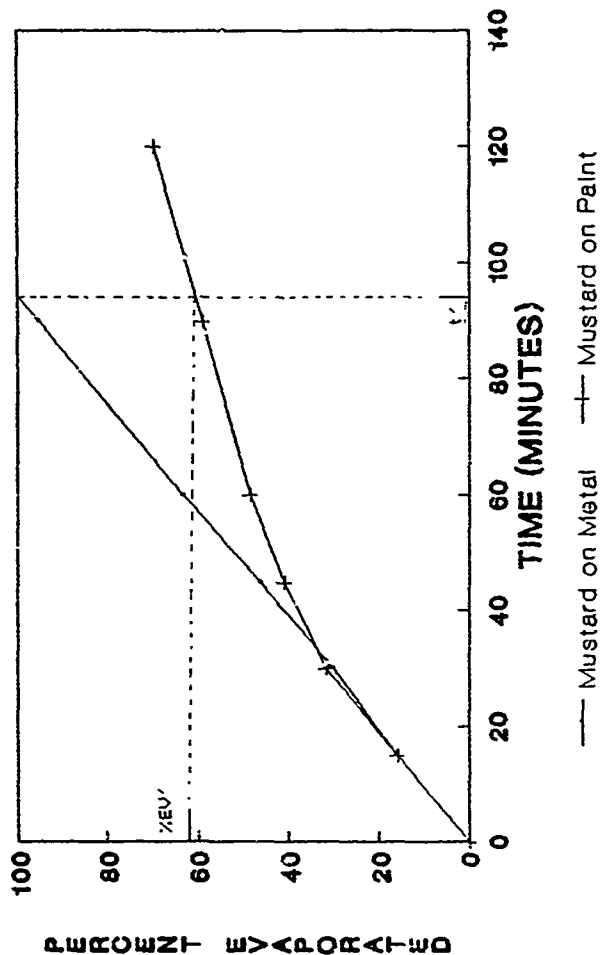


Figure 3. Evaporation of Mustard From Metal vs. Alkyd Resin Paint:
Determination of t' and $\%EV'$.

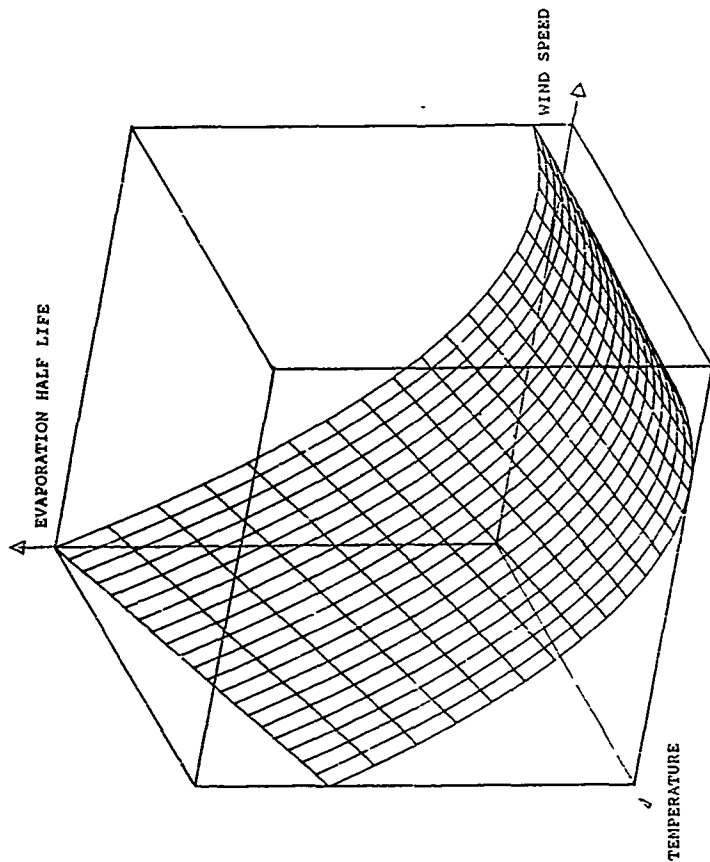


Figure 4. Evaporation Model of Mustard From Aged Paint as a Function of Temperature and Wind Speed.

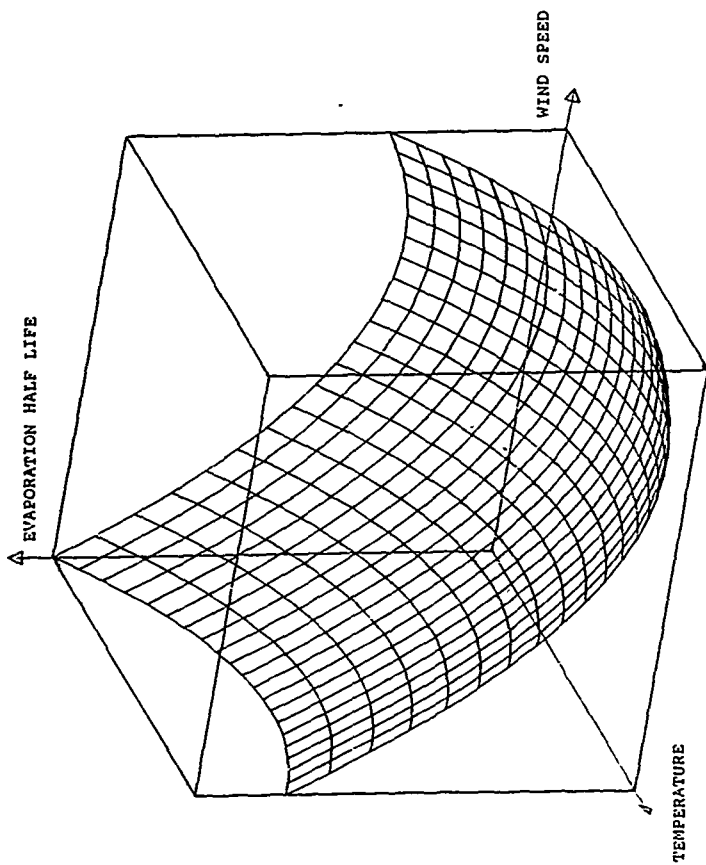


Figure 5. Evaporation Model of Mustard From Fresh Point as a Function of Temperature and Wind Speed.

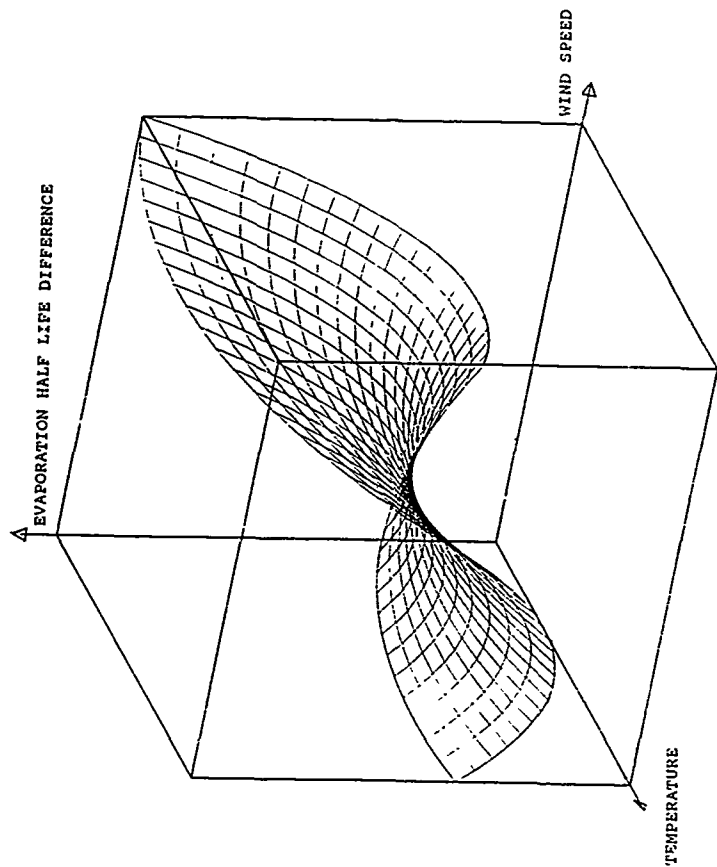


Figure 6. Graphical Subtraction of Aged Paint From Fresh Paint Model.

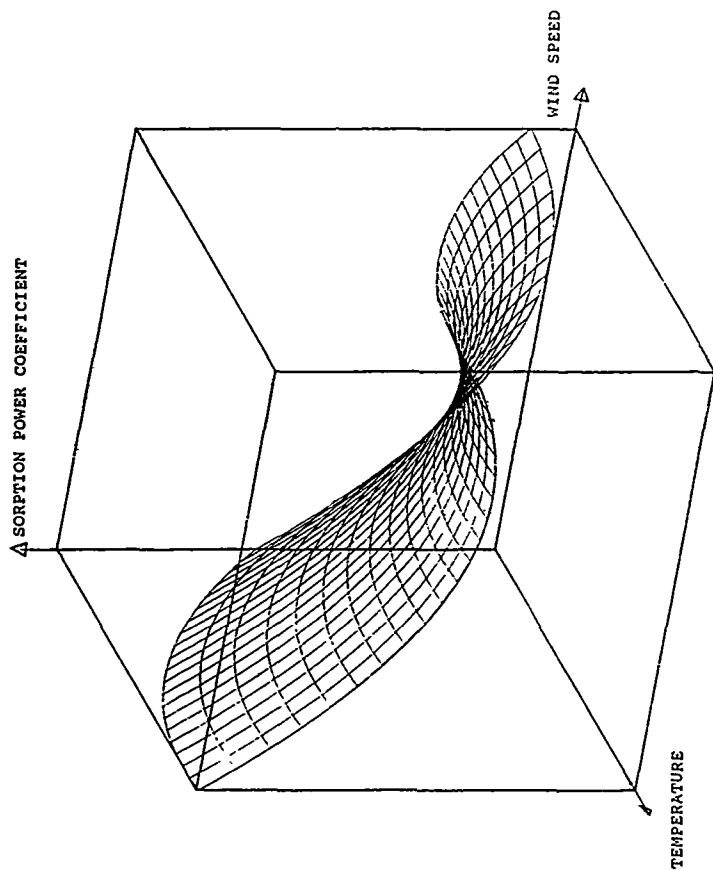


Figure 7. Paint Sorption Power Coefficient as a Function of Temperature and Wind Speed for Aged Paint Model.

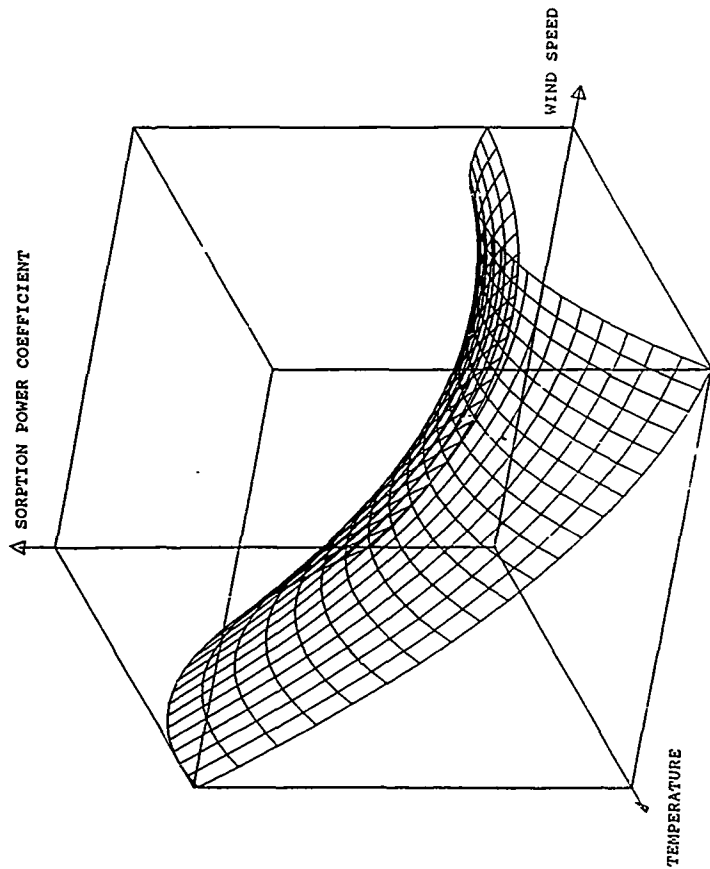


Figure 8. Paint Sorption Power Coefficient as a function of Temperature and Wind Speed for Fresh Paint Model.